Tess Eleonora Smidt

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Education and Training

Lawrence Berkeley Laboratory (Fall 2018 - Present)
Luis W. Alvarez Postdoctoral Fellow

University of California, Berkeley (Fall 2012 - Spring 2018)
Ph.D, Physics Awards Spring 2018
M.A., Physics Awarded Spring 2014
National Science Foundation Research Fellow (GPA: 3.8/4.0)
Advisor: Prof. Jeffrey B. Neaton
Subfield: Computational Condensed Matter Physics

Massachusetts Institute of Technology (Fall 2008 - Spring 2012)
S.B., Physics with minor in Architecture (GPA: 4.5/5.0)
Advisor: Prof. Janet Conrad
Subfield: Experimental and Computational Particle Physics

Research Interests:
Deep learning for science, materials design, procedural geometry

Computing tools: Density functional theory, high-performance computing, Python, scientific workflows, TensorFlow, PyTorch, CAD

Selected Coursework:
Deep Learning, Computational Geometry, Quantum Field Theory

Luis W. Alvarez Postdoctoral Fellow in Computing Sciences (Fall 2018 - Present)

Lawrence Berkeley Laboratory

- ***Awarded two year fellowship to pursue unrestricted, independent research in computational science.***
- ***Designing neural networks to generate novel atomic crystal structures.*** This will alleviate current bottlenecks in high-throughput computational materials discovery pipelines where searches are limited to databases of experimentally known materials.

Google Internship: Accelerated Science Team (Summer 2017 - Spring 2018)

- ***Designed and implemented a 3D-rotation-equivariant convolutional neural network in TensorFlow.*** How to create such a network had been an open question in deep learning for several years. Initiated project within the Accelerated Science team. Network can identify local features in different positions and orientations in 3D using network connectivity and filters that are compatible with representations of the group of 3D rotations. Network can accept scalars, vectors, and tensor fields as input and output. This network can be used to predict properties of molecules and crystals given the coordinates of constituent atoms as input. Model is available on GitHub.
- ***Created machine learning models to predict quantities relevant for catalysis.*** Models interpolate between computationally expensive quantum mechanical calculations performed by academic collaborators. Used variety of model architectures and hyperparameter searches to train models that could predict relevant quantities within an order of magnitude of quantum mechanical calculation accuracy with simple featurization. Identified several data features that impact hydrogen adsorption energy.

Graduate Research

- ***Helped discover two new classes of crystals.*** Worked with synthetic chemists to characterize a new class of self-assembled crystals with exotic 2D optical and electronic properties in a 3D form. Operated one of the world's strongest magnets and most intense x-ray sources to characterize a new

quantum magnetic material. Predicted the stability of a new class of quantum magnetic crystals. Simulated crystal growth using Metropolis-Hastings algorithm.

- ***Performed an automated computational search for ferroelectrics -- materials used for tunable capacitors and non-volatile RAM.*** Integrated crystal structure databases, symmetry tools, workflow software, density functional theory, visualization, and analysis. Workflow and analysis tools contributed to atomate and pymatgen python packages. First dataset of 150 high-quality ferroelectric candidates in preparation for open submission.
- ***Designed algorithms for generating new atomic systems from geometric primitives.*** Created a geometric algorithm to coat curved surfaces with a graphene-like structure using anisotropic Delaunay triangulations. Used geometric models to correlate structural deformations with changes in electronic properties of atoms that form low-dimensional chains of connected polyhedra.
- ***Created tools for improving synthesis reproducibility.*** To augment paper notebooks used by synthesis groups, I created a lab database system to connect material synthesis methods with experimental data.

Undergraduate Research

- Designed a 40'-long light detection system structure for a 70-ton liquid argon neutrino detector. This structure was installed in 2013.
- Designed a new neutrino source. Simulated particle physics, nuclear physics, and heat transfer.
- Conducted preliminary feasibility study of whether a new Higgs boson interaction type could be detected at the Large Hadron Collider.

Mischief

- ***The Lunch Experiment*** -- Developed an automated system that invited grad students from different departments to group lunches. Organized over 150 "randomized controlled lunches" and grew a community of more than 400 grad students from 50 departments. ***(Summer 2015 - Spring 2016)***
- ***Cosmic Ray Chandeliers*** -- Funded by MIT to design, fabricate, and install two 4' tall chandeliers that illuminate upon detecting cosmic ray muons – particles created when nuclei from outer space bombard Earth's atmosphere. See http://www.blondegeek.net/cosmicray/ ***(Fall 2010 - Spring 2011)***
- ***blondegeek.net*** -- Launched t-shirt company in Summer 2006 at age 16. Designed web site, created customer and product databases and wrote inventory management software. During ten years of business, designed and sold thousands of shirts. ***(2006-2016)***

Publications In Preparation

T. Smidt, S. Reyes-Lillo, A. Jain, J. B. Neaton, *An Automatically Curated First-Principles Database of Ferroelectrics*, Submitted to Nature Scientific Data (2018). In revision (2019).

T. Smidt, S. Griffin, J. B. Neaton, *Ab initio Studies of Structural and Energetic Trends in the Harmonic Honeycomb Iridates*, In preparation for submission to Physical Review: B (2019).

M. Collins, **T. Smidt** et al., *A Self-Assembled Hybrid Chalcogenide Exhibits 2D Semiconducting Properties in its Bulk Crystal*, In revision (2019).

Publications and Patent

N. Thomas, **T. Smidt** et al., Tensor field networks: Translation- and 3D rotation- equivariant convolutional neural networks. arXiv:1802.08219 (2018).

Kiran Mathew et al., *Atomate: A High-Level Interface to Generate, Execute, and Analyze Computational Materials Science Workflows*, Computational Materials Science, Volume 139, 140-152 (2017).

J.N. Hohman, M. Collins, and **T. Smidt**, *Mithrene and methods of fabrication of mithrene*, (2017). International Patent App. PCT/US20l7/045609. Filed August 4, 2017.

K. Modic, **T. Smidt,** I. Kimchi et al., *Realization of a three-dimensional spin-anisotropic harmonic honeycomb iridate*, Nature Communications 5 (2014). (arXiv:1402.3254)

T. Briese et al., *Testing of Cryogenic Photomultiplier Tubes for the MicroBooNE Experiment*, Journal of Instrumentation 8, T07005 (2013). (arXiv:1304.0821)

A. Bungau et al. *Proposal for an electron antineutrino disappearance search using high-rate 8Li production and decay,* Physical Review Letters 109, 141802 (2012). (arXiv:1205.4419)

A. Bungau, **T. Smidt** et al., *Simulations of Pion Production in the DAEδALUS Target*, Conference proceedings for the International Particle Accelerator Conference (2012). (arXiv:1205.4419)

L. Bugel et al., *Demonstration of a Lightguide Detector for Liquid Argon TPCs*, Nuclear Instruments and Methods in Physics Research Section A (2011). (arXiv:1101.3013)

J. Alonso et al., *Expression of Interest for a Novel Search for CP Violation in the Neutrino Sector: DAEdALUS*, (2010). (arXiv:1006.0260)

Workshops

Rising Stars in Computational and Data Science (April 8-10, 2019)
ICES @ UT Austin Austin, TX

Invited Talks (Upcoming and Previous)

MolKin 2019: Molecular Kinetics and Sampling, Design and Machine Learning (June 19-21, 2019)
Freie Universität Berlin, Germany Berlin, Germany

TGDA @ OSU TRIPODS Center Workshop on "Structure in the Micro-world" (May 28-31, 2019)
Ohio State University Columbus, OH

DISC @ Lehigh TRIPODS+X Conference (May 22-24, 2019)
Lehigh University Bethlehem, PA

Machine Learning in Nonlinear Physics and Mechanics (March 4-9, 2019)
American Physical Society (APS) March Meeting Boston, MA

Molecular and Electronic Structure Theory Meets Data Science Session (March 1, 2019)
Society for Industrial and Applied Mathematics (SIAM) Spokane, WA
Computational Science and Engineering Conference

Molecular Foundry Seminar, Lawrence Berkeley Laboratory (October 23, 2018)

Lawrence Berkeley Laboratory — Berkeley, CA

Title: Toward the Systematic Generation of Hypothetical Atomic Structures: Neural Networks and Geometric Motifs

Machine Learning for Molecules and Materials Workshop — (December 8, 2018)

Conference on Neural Information Processing Systems (NeurIPS) — Montreal, Canada

Title: Tensor field networks: rotation-, translation-, and permutation-equivariant convolutional neural networks for 3D point clouds

ML4Science Workshop — (September 4, 2018)

Lawrence Berkeley Laboratory — Berkeley, CA

Title: ML for Atomic Systems: Challenges and Applications